

# Wave equations for determining energy-level gaps of quantum systems

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An differential equation for wave functions is proposed, which is equivalent to Schrödinger's wave equation and can be used to determine energy-level gaps of quantum systems. Contrary to Schrödinger's wave equation, this equation is on 'bipartite' wave functions. It is shown that those 'bipartite' wave functions satisfy all the basic properties of Schrödinger's wave functions. Further, it is argued that 'bipartite' wave functions can present a mathematical expression of wave-particle duality. This provides an alternative approach to the mathematical formalism of quantum mechanics.

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In the most general form, Heisenberg's equation [1] and Schrödinger's equation [2] can be written as follows

$$i\hbar \frac{\partial \hat{O}(t)}{\partial t} = [\hat{O}(t), \hat{H}], \quad (1)$$

and

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle, \quad (2)$$

respectively, where  $\hat{H}$  is the Hamiltonian of the system. As is well known, these two forms for the equations of motion of quantum mechanics are equivalent. Of these, the Schrödinger form seems to be the more useful one for practical problems, as it provides differential equations for wave functions, while Heisenberg's equation involves as unknowns the operators forming the representative of the dynamical variable, which are far more numerous and therefore more difficult to evaluate than the Schrödinger unknowns.

On the other hand, determining energy levels of various dynamic systems is an important task in quantum mechanics, for this solving Schrödinger's wave equation is a usual way. Recently, Fan and Li [3] showed that Heisenberg's equation can also be used to deduce the energy level of some systems. By introducing the conception of invariant 'eigen-operator', they derive energy-level gap formulas for some dynamic Hamiltonians. However, their 'invariant eigen-operator' equation involves operators as unknowns, as similar to Heisenberg's equation, and hence is also difficult to evaluate in general.

In this article we propose an differential equation for wave functions, which can be used to determine energy-level gaps of quantum systems and is mathematically equivalent to Schrödinger's wave equation, that is, they can be solved from one another. Contrary to

Schrödinger's wave equation, this equation is on 'bipartite' wave functions. It is shown that those 'bipartite' wave functions satisfy all the basic properties of Schrödinger's wave functions. In particular, it is argued that 'bipartite' wave functions can present a mathematical expression of wave-particle. This provides an alternative approach to the mathematical formalism of quantum mechanics.

For convenience, we deal with the quantum system of a single particle. Note that the Hamiltonian for a single particle in an external field is

$$\hat{H}(\vec{x}) = -\frac{\hbar^2}{2m} \nabla_{\vec{x}}^2 + U(\vec{x}), \quad (3)$$

where  $\nabla_{\vec{x}}^2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$ ,  $U(\vec{x})$  is the potential energy of the particle in the external field, and  $\vec{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ . Then, Schrödinger's wave equation for a single particle in an external field is

$$i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} = \hat{H}(\vec{x})\psi(\vec{x}, t) = -\frac{\hbar^2}{2m} \nabla_{\vec{x}}^2 \psi(\vec{x}, t) + U(\vec{x})\psi(\vec{x}, t). \quad (4)$$

On the other hand, let  $\psi(\vec{x}, t)$  and  $\varphi(\vec{x}, t)$  both satisfy Eq.(4). Then we have

$$\begin{aligned} i\hbar \frac{\partial (\psi(\vec{x}, t)\varphi^*(\vec{y}, t))}{\partial t} &= i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} \varphi^*(\vec{y}, t) + i\hbar \frac{\partial \varphi^*(\vec{y}, t)}{\partial t} \psi(\vec{x}, t) \\ &= [\hat{H}(\vec{x})\psi(\vec{x}, t)] \varphi^*(\vec{y}, t) \\ &\quad - [\hat{H}(\vec{y})\varphi(\vec{y}, t)]^* \psi(\vec{x}, t) \\ &= (\hat{H}(\vec{x}) - \hat{H}(\vec{y})) (\psi(\vec{x}, t)\varphi^*(\vec{y}, t)). \end{aligned}$$

This leads to the following wave equation

$$i\hbar \frac{\partial \Psi(\vec{x}, \vec{y}; t)}{\partial t} = (\hat{H}(\vec{x}) - \hat{H}(\vec{y})) \Psi(\vec{x}, \vec{y}; t), \quad (5)$$

where  $\Psi(\vec{x}, \vec{y}; t) \in L_{\vec{x}, \vec{y}}^2$ . Contrary to Schrödinger's wave equation Eq.(4) for 'one-partite' wave functions  $\psi(\vec{x}) \in L_{\vec{x}}^2$ , the wave equation Eq.(5) is an differential equation for 'bipartite' wave functions  $\Psi(\vec{x}, \vec{y})$ , which, replacing

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$\hat{H}(\vec{x}) + \hat{H}(\vec{y})$  by  $\hat{H}(\vec{x}) - \hat{H}(\vec{y})$ , is also different from Schrödinger's wave equation for two particles.

Since

$$\frac{\partial |\Psi(\vec{x}, \vec{y}; t)|^2}{\partial t} = 2i \text{Re} \left[ \Psi^*(\vec{x}, \vec{y}; t) \frac{\partial \Psi(\vec{x}, \vec{y}; t)}{\partial t} \right],$$

it is concluded from Eq.(5) that

$$\frac{\partial}{\partial t} \int |\Psi(\vec{x}, \vec{y}; t)|^2 d^3\vec{x} d^3\vec{y} = 0. \quad (6)$$

This implies that Eq.(5) preserves the probability density  $|\Psi(\vec{x}, \vec{y}; t)|^2 d^3\vec{x} d^3\vec{y}$  with respect to time and means that, if this wave function  $\Psi$  is given at some instant, its behavior at all subsequent instants is determined.

By Schmidt's decomposition theorem [4], for every  $\Psi(\vec{x}, \vec{y}) \in L^2_{\vec{x}, \vec{y}}$  there exist two orthogonal sets  $\{\psi_n\}$  and  $\{\varphi_n\}$  in  $L^2_{\vec{x}}$  and  $L^2_{\vec{y}}$  respectively, and a sequence of positive numbers  $\{\mu_n\}$  satisfying  $\sum_n \mu_n^2 < \infty$  so that

$$\Psi(\vec{x}, \vec{y}) = \sum_n \mu_n \psi_n(\vec{x}) \varphi_n^*(\vec{y}). \quad (7)$$

Then, it is easy to check that

$$\Psi(\vec{x}, \vec{y}; t) = \sum_n \mu_n \psi_n(\vec{x}, t) \varphi_n^*(\vec{y}, t)$$

satisfies Eq.(5) with  $\Psi(\vec{x}, \vec{y}; 0) = \Psi(\vec{x}, \vec{y})$ , where both  $\psi_n(\vec{x}, t)$  and  $\varphi_n(\vec{y}, t)$  satisfy Eq.(4) with  $\psi_n(\vec{x}, 0) = \psi_n(\vec{x})$  and  $\varphi_n(\vec{y}, 0) = \varphi_n(\vec{y})$ , respectively. Hence, the wave equation Eq.(5) can be solved mathematically from Schrödinger's wave equation.

Given  $\psi \in L^2_{\vec{x}}$ , for every  $t \geq 0$  define operators  $\varrho_t$  on  $L^2_{\vec{x}}$  by

$$(\varrho_t \varphi)(\vec{x}) = \int \Psi(\vec{x}, \vec{y}; t) \varphi(\vec{y}) d^3\vec{y}, \quad (8)$$

where  $\Psi(\vec{x}, \vec{y}; t)$  is the solution of Eq.(5) with  $\Psi(\vec{x}, \vec{y}; 0) = \psi(\vec{x}) \psi^*(\vec{y})$ . It is easy to check that

$$i \frac{\partial \varrho_t}{\partial t} = [H, \varrho_t], \quad \varrho_0 = |\psi\rangle\langle\psi|. \quad (9)$$

This is just Schrödinger's equation in the form of density operators. Hence, Schrödinger's wave equation is a special case of the wave equation Eq.(5) with initial values of product form  $\Psi(\vec{x}, \vec{y}; 0) = \psi(\vec{x}) \psi^*(\vec{y})$ . Therefore, the wave equation Eq.(5) is mathematically equivalent to Schrödinger's wave equation.

In the sequel, we consider the problem of stationary states. Let  $\psi_n$  be the eigenfunctions of the Hamiltonian operator  $\hat{H}$ , i.e., which satisfy the equation

$$\hat{H}(\vec{x}) \psi_n(\vec{x}) = E_n \psi_n(\vec{x}), \quad (10)$$

where  $E_n$  are the eigenvalues of  $\hat{H}$ . Correspondingly, the wave equation Eq.(5)

$$\begin{aligned} i\hbar \frac{\partial \Psi(\vec{x}, \vec{y}; t)}{\partial t} &= (\hat{H}(\vec{x}) - \hat{H}(\vec{y})) \Psi(\vec{x}, \vec{y}; t) \\ &= (E_n - E_m) \Psi(\vec{x}, \vec{y}; t) \end{aligned}$$

with  $\Psi(\vec{x}, \vec{y}; 0) = \psi_n(\vec{x}) \psi_m^*(\vec{y})$ , can be integrated at once with respect to time and gives

$$\Psi(\vec{x}, \vec{y}; t) = e^{-i\frac{1}{\hbar}(E_n - E_m)t} \psi_n(\vec{x}) \psi_m^*(\vec{y}). \quad (11)$$

Since  $\{\psi_n(\vec{x})\}$  is a complete orthogonal set in  $L^2_{\vec{x}}$ , it is concluded that  $\{\psi_n(\vec{x}) \psi_m^*(\vec{y})\}$  is a complete orthogonal set in  $L^2_{\vec{x}, \vec{y}}$ . Then, for every  $\Psi(\vec{x}, \vec{y}) \in L^2_{\vec{x}, \vec{y}}$  there exists a unique set of numbers  $\{c_{n,m}\}$  satisfying  $\sum_{n,m} |c_{n,m}|^2 < \infty$  so that

$$\Psi(\vec{x}, \vec{y}) = \sum_{n,m} c_{n,m} \psi_n(\vec{x}) \psi_m^*(\vec{y}). \quad (12)$$

Hence, for  $\Psi(\vec{x}, \vec{y}; 0) = \sum_{n,m} c_{n,m} \psi_n(\vec{x}) \psi_m^*(\vec{y})$  we have that

$$\Psi(\vec{x}, \vec{y}; t) = \sum_{n,m} c_{n,m} e^{-i\frac{1}{\hbar}(E_n - E_m)t} \psi_n(\vec{x}) \psi_m^*(\vec{y}) \quad (13)$$

for  $t \geq 0$ . Now, if  $\Psi(\vec{x}, \vec{y}) \in L^2_{\vec{x}, \vec{y}}$  is an eigenfunction of the operator  $\hat{H}(\vec{x}) - \hat{H}(\vec{y})$ , i.e., which satisfies the equation

$$(\hat{H}(\vec{x}) - \hat{H}(\vec{y})) \Psi(\vec{x}, \vec{y}) = \lambda \Psi(\vec{x}, \vec{y}), \quad (14)$$

where  $\lambda$  is an associated eigenvalue, then  $\Psi(\vec{x}, \vec{y}; t) = e^{-i\frac{1}{\hbar}\lambda t} \Psi(\vec{x}, \vec{y})$  satisfies Eq.(5) and consequently, it is concluded from Eq.(13) that  $\lambda = E_n - E_m$  is an energy-level gap of the system. Thus, the wave equation Eq.(5) can be used to determine energy-level gaps of the system.

It is well known that the basis of the mathematical formalism of quantum mechanics lies in the proposition that the state of a system can be described by a definite Schrödinger's wave function of coordinates [5, 6]. The square of the modulus of this function determines the probability distribution of the values of the coordinates [7]. Since the wave equation Eq.(5) is mathematically equivalent to Schrödinger's wave equation, it seems that the state of a quantum system also can be described by a definite 'bipartite' wave function of Eq.(5), of which the physical meaning is that the 'bipartite' wave functions of stationary states determine energy-level gaps of the system.

In fact, we can make the general assumption that if the measurement of an observable  $\hat{O}$  for the system in the 'bipartite' state corresponding to  $\Psi$  is made a large number of times, the average of all the results obtained will be

$$\langle \hat{O} \rangle_{\Psi} = \text{Tr} [\varrho_{\Psi}^{\dagger} \hat{O} \varrho_{\Psi}], \quad (15)$$

where  $\varrho_{\Psi}$  is an operator on  $L^2$  associated with  $\Psi$  defined by  $(\varrho_{\Psi} \varphi)(\vec{x}) = \int \Psi(\vec{x}, \vec{y}) \varphi(\vec{y}) d^3\vec{y}$  for every  $\varphi \in L^2$ , provided  $\Psi$  is normalized. That is, the expectation value of an observable  $\hat{O}$  in the 'bipartite' state corresponding to  $\Psi$  is determined by Eq.(15). It is easy to check that if  $\Psi(\vec{x}, \vec{y}) = \psi(\vec{x}) \psi^*(\vec{y})$ , then

$$\langle \hat{O} \rangle_{\Psi} = \langle \psi | \hat{O} | \psi \rangle. \quad (16)$$

This concludes that our expression Eq.(15) agrees with the interpretation of Schrödinger's wave functions for calculating expectation values of any chosen observable.

Moreover, 'bipartite' wave functions can present a mathematical expression of wave-particle duality. Let us discuss the double-slit experiment [8]. Let  $\phi_1$  and  $\phi_2$  be two Schrödinger's wave functions of the particle arrival through slit 1 and slit 2, respectively. Then, the associated 'bipartite' wave function of the particle arrival through both slit 1 and slit 2 can be either

$$\Psi_W(\vec{x}, \vec{y}) = (\phi_1(\vec{x}) + \phi_2(\vec{x})) (\phi_1^*(\vec{y}) + \phi_2^*(\vec{y})), \quad (17)$$

or

$$\Psi_P(\vec{x}, \vec{y}) = \phi_1(\vec{x})\phi_1^*(\vec{y}) + \phi_2(\vec{x})\phi_2^*(\vec{y}). \quad (18)$$

A single particle described by  $\Psi_W$  behaves like waves, while by  $\Psi_P$  like particles. This is so because for position, by (15) we have

$$\langle \hat{x} \rangle_{\Psi_W} \propto |\phi_1(\vec{x}) + \phi_2(\vec{x})|^2, \langle \hat{x} \rangle_{\Psi_P} \propto |\phi_1(\vec{x})|^2 + |\phi_2(\vec{x})|^2$$

respectively. On the other hand,  $\Psi_P$  is a 'bipartite' entangled state [9], which means that a single particle can entangle with itself [10], as similar to the fact that each photon can interfere with itself, as shown in Ref. [6]. Then, it is concluded that a single particle behaves like waves when it interfere with itself, while like particle when entangle with itself. Thus, wave-particle duality is just the complementarity of interference and entanglement for a single particle. A more detail on this issue will

be given in the future. Since entanglement plays a crucial role in quantum communication, cryptograph, and computation [11], we may expect that the entanglement of a *single* particle will play an important role in quantum information [12].

We would like to mention that Eq.(5) have been presented by Landau and Lifshitz [13] giving the change in the density matrix with time, similar to the Schrödinger's wave equation. However, we regard Eq.(5) as a wave equation but not a equation for density functions. This is the key point which is distinct from [13]. As shown above, Eq.(5) is a suitable form for motion of quantum mechanics as a 'bipartite' wave equation.

In summary, we present an differential equation for wave functions, which is equivalent to Schrödinger's wave equation and can be used to determine energy-level gaps of the system. Contrary to Schrödinger's wave equation, this equation is on 'bipartite' wave functions. It is shown that those 'bipartite' wave functions satisfy all the basic properties of Schrödinger's wave functions. Further, it is argued that 'bipartite' wave functions can present a mathematical expression of wave-particle duality. Our results shed considerable light on the mathematical basis of quantum mechanics.

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- [1] W.Heisenberg, Z. Physik **33**, 879(1925).
  - [2] E.Schrödinger, Ann.Physik **79**, 36(1926).
  - [3] H.-Y.Fan and C.Li, Phys.Lett.A **321**, 75(2004).
  - [4] E.Schmidt, Math.Ann.**63**, 433(1907).
  - [5] J.von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, 1955).
  - [6] P.A.M.Dirac, *The Principles of Quantum Mechanics* (Fourth edition, Oxford University Press, Oxford, 1958).
  - [7] M.Born, Z.Physik **38**, 803(1926).
  - [8] R.P.Feynman and A.R.Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, Inc., 1965).
  - [9] A.Einstein, B.Podolsky, and N.Rosen, Phys. Rev. **47**, 777(1935); E.Schrödinger, Naturwissenschaften **23**, 807(1935); R.Werner, Phys.Rev.A **40**, 4277(1989).
  - [10] S.J.van Enk, Phys.Rev.A **72**, 064306(2005), and references therein.
  - [11] C.H.Bennett, *et al*, Phys.Rev.Lett.**70**, 1895(1993); N.Gisin, G.Ribordy, W.Tittle, and H.Zbinden, Rev. Mod. Phys.**74**, 145(2002); M.Nielsen and I.Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
  - [12] S.A.Babichev, *et al*, Phys.Rev.Lett.**92**, 193601(2004), and references therein.
  - [13] L.D.Landau and E.M.Lifshitz, *Quantum Mechanics (Non-relativistic Theory)* (Third edition, Pergamon Press, Oxford, 1977), 38-41.